Loïc Dumortier, PhD

+32 494 16 64 53 | Cologne, Germany | loicdumortier@proton.me | linkedin.com/in/dumortier-loic

Computational chemist with a PhD in Physics, specialized in machine-learning interatomic potentials, reactive force-field development, high-throughput quantum chemistry and large-scale atomistic modeling. Combines an analytical chemistry foundation with physics-level rigor.

Work Experience

Research Scientist 2025 — 2026
German Aerospace Center (DLR) *Cologne, Germany*
- Led and delivered cross-functional computational chemistry and materials science projects in collaboration with industry partners
- Engineered robust data pipelines using state-of-the-art molecular modeling methods for high-throughput surface detection, resulting in the identification and characterization of unknown stable high-index surfaces.

Doctoral Researcher 2023 — 2025
Center for Molecular Modeling *Ghent, Belgium*
- Developed scalable empirical reactive force fields and machine learning potentials through novel optimization frameworks, resulting in successfully modeling alumina and hydrated silicate ionic liquids with a 5-10x simulation speed-up

Research Engineer 2020 — 2023
IFP Energies Nouvelles *Rueil-Malmaison, France*
- Optimized ReaxFF reactive force field parameters through the successful development and deployment of machine learning algorithms, allowing accurate modeling of complex alumina systems in a catalytic context
- Extracurricular: Board-member of the doctoral association, successfully organizing network events, study trips and PhD onboarding

Research Intern 2019 — 2019
Institut Laue Langevin & European Synchrotron Radiation Facility *Grenoble, France*
- Advanced soft matter studies by successfully identifying water contents from molecular dynamics simulations through 3D imaging machine learning approaches, resulting in a first-author publication

Education

Ghent University Ghent, Belgium
Doctor of Philosophy in Physics *2020 — 2025*
- Title: Model-Informed Training Data Curation for Reactive All-Atom Potentials
- Research Group: Center for Molecular Modeling

IFP School Rueil-Malmaison, France
Doctoral Training Program *2020 — 2023*
- Coursework focused on energy economics, refining processes, and petroleum products

Ghent University Ghent, Belgium
Master of Science in Analytical Chemistry (Summa Cum Laude) *2014 — 2020*
- Thesis: Development of advanced 2D/3D data analysis methods for on-the-fly scanning XRF experiments
- Extracurricular: Student Representative, Faculty Representative, Chemistry PR Representative

Technical Skills & Competencies

- **Core Competencies**: Machine Learning Potentials, Force Field Development, HPC, Molecular Dynamics, DFT, Materials Science, X-Ray Fluorescence, X-Ray Diffraction, Chemometrics
- **Programming & Tools**: Python, Git, Unix, Docker, OpenMM, VASP, FHI-AIMS, LAMMPS, pymatgen, ASE, MACE, PyTorch, Numpy, Pandas, Scikit-learn
- **Languages**: English (C1), French (C1), Dutch (Native), German (A2, learning)

Grants & Awards

Awardee, Tier-1 Compute Grant (Flemish Supercomputing Center) 2023 — 2023
- Secured and managed 2.25 million CPU hours and 27,000 GPU hours for large-scale computational research

First Place, ParAMS Challenge Winner (Software for Chemistry and Materials) 2022 — 2022
- Recognized globally for innovations in advanced molecular simulation and force field optimization